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Mechanism of temperature dependence of the magnetic anisotropy energy in ultrathin Cobalt and Nickel films

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Temperature dependent FMR-measurements of Ni and Co films are analysed using a microscopic theory for ultrathin metallic systems. The mechanism governing the temperature dependence of the magnetic anisotropy energy is identified and discussed. It is reduced with increasing temperature. This behavior is found to be solely caused by magnon excitations.

I. INTRODUCTION

Research on ultrathin films has been growing considerably over the last two decades due to their technical importance and the increasing ability to grow high-quality film samples. When dealing with systems of reduced dimensionality it is important to take into account the influence of magnetic anisotropies. Formally being a prerequisite for finite temperature magnetism[1] they also play a crucial role in reorientation transitions as functions of film thickness, temperature, or an external magnetic field[2].

In this work we present a microscopic quantum mechanical model to describe the temperature dependence of the magnetic anisotropies of ultrathin Ni and Co films. As the dominant anisotropy terms in these transition metals we take into account a second order lattice anisotropy and dipolar coupling. We are able to fit experimental data obtained by the ferromagnetic resonance technique (FMR)[3,4] with our model, which is based on a Heisenberg exchange between localized magnetic moments. The main result will be that the T-dependence of the anisotropy is solely due to magnon excitations rather than to other mechanisms as, e.g., thermal expansion or phononic interactions. The isolation of the magnon effect is of course not possible when describing the films with the classical (T=0-) Landau-Lifshitz equations in which the (effective) anisotropy parameters have to be fitted at each given temperature[4]. Temperature is taken into account explicitly by the so-called stochastic Landau-Lifshitz-Gilbert (LLG) equation[5]. However we will introduce in the following an alternative approach based on a quantum mechanical description of the film system and an explicite consideration of magnon excitations using a Heisenberg model containing atomistic anisotropy terms.

II. THEORETICAL DESCRIPTION

The Hamiltonian of our microscopic model reads

$$H = -\sum_{ij} J_{ij}\mathbf{S}_i\mathbf{S}_j - \sum_i g_J\mu_B\mathbf{B}_0\mathbf{S}_i - \\ -\sum_i K_2 S_{iz'}^2 + \sum_{ij} g_0\left(\frac{1}{r_{ij}^3}\mathbf{S}_i\mathbf{S}_j - \frac{3}{r_{ij}^5}(\mathbf{S}_i\mathbf{r}_{ij})(\mathbf{S}_j\mathbf{r}_{ij})\right) \qquad (1)$$

The first term describes Heisenberg coupling J_{ij} between magnetic spin moments $\mathbf{S}_i$ at the sites of a monolayer. It represents the largest energy scale in the problem and is responsible for the magnetism in the system. A film thickness beyond monolayer is effectively absorbed into the nearest neighbor exchange parameter J to which we restrict ourselves. J is chosen such that the monolayer magnetic moment equals that of the multilayer film at room temperature ($T_C^{Ni_7} = 410$ K, $T_C^{Co_2} = 400$ K). The second term contains an external magnetic field $\mathbf{B}_0$ in arbitrary direction with the Landé factor g_J and the Bohr magneton μ_B. The third and fourth term constitute lattice anisotropy and dipolar interaction, respectively, the latter leading to shape anisotropy. K_2 and g_0 are microscopic anisotropy parameters, $S_{iz'}$ is the z'-component of $\mathbf{S}_i$ perpendicular to the film plane, and $\mathbf{r}_{ij}$ is the vector between lattice sites i and j. The shape anisotropy favors in-plane orientation and the lattice anisotropy can favor in-plane ($K_2 < 0$) or out-of-plane ($K_2 > 0$) orientation of the magnetization.

The main idea of the method that we used in order to solve (1) is discussed in Ref.[2]. The exchange terms are decoupled using the standard Tyablikov (RPA) approximation. The crucial point is to find a reasonable decoupling of the lattice anisotropy terms in the equation of motion for the spin Green function $\langle\langle S_i^+; S_j^-\rangle\rangle$ given an *arbitrarily* oriented external magnetic field. This problem is solved by performing a coordinate transformation $(x', y', z') \rightarrow (x, y, z)$. More precisely one self-consistently rotates the initial coordinate system defined by a z'-axis parallel to the film normal such that the z-axis of the new reference frame has the direction of the magnetization. Then an Anderson-Callen decoupling to

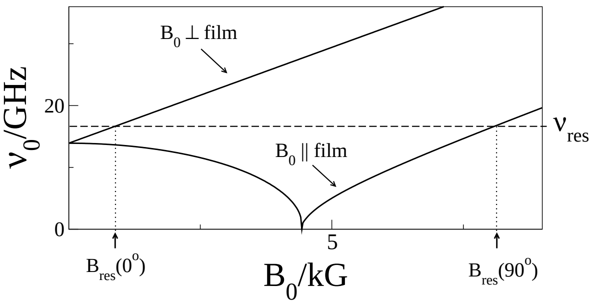

FIG. 1: Resonance frequency as a function of the external magnetic field applied parallel ($\theta_{B_0} = 90°$) and perpendicular ($\theta_{B_0} = 0°$) to the film plane (monolayer). The resonance fields can be detected by an FMR experiment. Parameters: $T = 0,\ K_2 = 10\mu_B$kG, $g_0 = 0$.

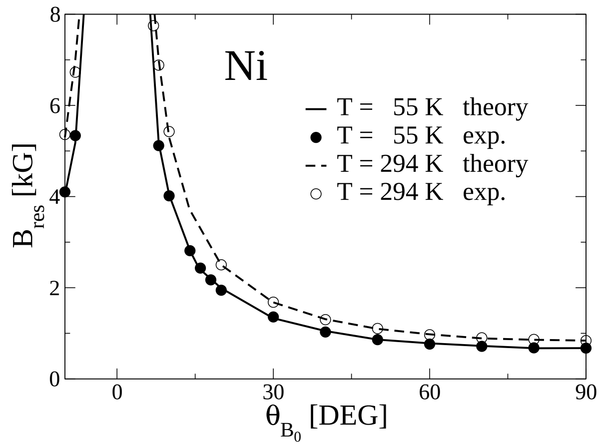

FIG. 2: Resonance field of Nickel at $T = 55$K and at $T = 294$K as a function of the orientation of the external magnetic field. Circles: experimental data from Ni_7/Cu(001). Lines connect theoretical fit points. S=1, $K_2 = 3.0\mu_B$kG, $g_0 = 4.5\mu_B$kG, $J = 30$meV.

the K_2-terms is applied[6]. The results for the magnetization components obtained by this approach compare very well with corresponding QMC calculations[2]. We have improved the theoretical treatment in the meantime by taking into account additional Green functions, namely all combinations of $\langle\langle S_i^{+,-}; S_j^{+,-}\rangle\rangle$, as was proposed in Ref.[7]. This improved theory ensures correct softening properties of the uniform spin wave mode and also agrees nicely with the QMC results. Furthermore the dipole term in (1) is treated in the RPA approximation and only the uniform ($\mathbf{q} \to 0$) contribution is considered as the non-uniform terms are negligible compared to contributions from the much larger Heisenberg exchange.

A more detailed and general account of our method (e.g. the explicit extension to the multilayer case) will be presented elsewhere. We summarize only the essential output here: solving for the spin Green functions yields weights $\chi_\alpha(\mathbf{q})$ and excitation energies $E_\alpha(\mathbf{q}) = \hbar\omega_\alpha(\mathbf{q})$ which in turn give the average magnon occupation number

$$\varphi(T) = \frac{1}{N}\sum_q \sum_\alpha \frac{\chi_\alpha(q)}{e^{\beta E_\alpha(q)} - 1}\ . \qquad (2)$$

The two terms of the sum over α describe the single-magnon excitations of the system for a given wave vector q, namely magnon creation and magnon annihilation. The magnetization (in the rotated frame) can then be computed from

$$\langle S_z\rangle = \frac{(1+\varphi)^{2S+1}(S-\varphi) + \varphi^{2S+1}(S+1+\varphi)}{(1+\varphi)^{2S+1} - \varphi^{2S+1}}\ . \qquad (3)$$

Our theory therefore allows for a self-consistent determination of the magnetization, i.e. temperature-dependent calculations. In addition the self-consistent determination of the rotation angle is achieved by requiring that S_z be a constant of the motion, $\frac{dS_z}{dt} = 0$, within the decoupling approximations we use in our theory. We point out that by properly rescaling the parameters our equations at $T = 0$ can actually be shown to reduce to the Landau-Lifshitz equations. A discussion of the important differences that appear for finite temperatures will be given elsewhere.

In our theory the anisotropies K_2 and g_0 influence the system solely via the *effective anisotropy* given by the temperature-dependent term

$$\tilde{K}_2(T) = \langle S_z\rangle(T)\,(2K_2C(T) - Dg_0)\ , \qquad (4)$$

$$C(T) = 1 - \frac{(S(S+1) - \langle S_z^2\rangle(T))}{2S^2}\ . \qquad (5)$$

Here the T-independent quantity D is some number depending on the lattice geometry. Note that our effective anisotropy $\tilde{K}_2$ is identical to the quantity M_{eff} commonly used within a Landau-Lifshitz description of FMR experiments[3]. Furthermore we exploit $\langle S_z^2\rangle(T) = S(S+1) - \langle S_z\rangle(T)(1 + 2\varphi(T))$. The temperature dependence of $\tilde{K}_2$ thus goes beyond a mere proportionality to $\langle S_z\rangle(T)$ due to the occurence of the higher order T-dependent correlation function $\langle S_z^2\rangle(T)$.

The experimental data have been obtained using FMR measurements[3,4]. This technique probes the uniform spin wave mode $\omega(\mathbf{q} = \mathbf{0})$ of a magnetic sample. An external field is tuned for a given probe frequency $\nu_0 = \omega(\mathbf{q} = \mathbf{0})/2\pi$ until resonance occurs at $B_{\rm res}(\theta_{B_0})$, with θ_{B_0} being the angle between the magnetic field and the normal to the filmplane. This is illustrated in Fig. 1.

Using the temperature dependent effective anisotropy (4) we can now fit the experimental data. We can thus check if the temperature dependence of the effective anisotropy is due to spin wave excitations which are considered explicitly in our model (1) or due to other (non-magnonic) effects which would manifest themselves in a temperature dependence of the parameters K_2 and g_0.

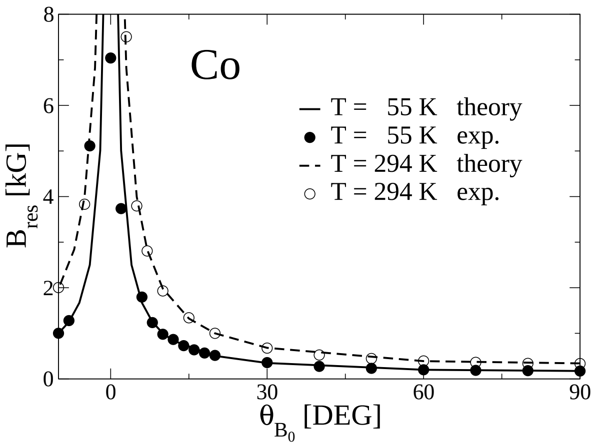

FIG. 3: Same as in Fig. 2 for Cobalt ($Cu_9/Co_2/Cu(001)$). Parameters: S=2.5, $K_2 = -20.25\mu_B$kG, $g_0 = 1.95\mu_B$kG, $J = 4.1$meV.

III. FIT TO EXPERIMENTS WITH NI AND CO FILMS

In the following we take $S = 1$ for Ni and $S = 2.5$ for Co due to different magnetic moments of the two metals[8]. The Landé factor is taken as $g_J = 2.1$ for both Ni and Co. The FMR microwave frequency was set to 9 GHz.

Fig. 2 and 3 show the comparison between the $B_{res}(\theta_{B_0})$-curves from theory and experimental data for a (subscript denotes the number of monolayers) $Cu_9/Co_2/Cu(001)$ and a $Ni_7/Cu(001)$ film system, respectively, at two different temperatures. In both cases the effective anisotropy favors the magnetization to lie within the film plane. There is quite good agreement at both temperatures over the whole range of angles θ_{B_0} for both films. At a given angle the resonance field increases with temperature.

It is important to note that the choice of the microscopic parameters K_2 and g_0 at a given temperature cannot be unambiguous as one easily sees from (4). However we took additionally into account the temperature dependence of the resonance field for a fixed angle $\theta_{B_0} = 90°$ as it is shown in Fig. 4. Due to the temperature dependent term which goes with K_2 in (4), namely $\langle S_z^2\rangle(T)$, the ambiguity is removed. Indeed it is still possible to accurately fit the experimental results with one set of (T-independent) parameters (K_2, g_0) for Ni and Co, respectively, over the whole temperature range. Furthermore in both cases the values of g_0S lie slightly above the result of an explicit evaluation of this quantity assuming point-like dipoles on the lattice sites for the given geometry[4] ($g_0S = 3.81\mu_B$kG). The conclusion we can draw is that the temperature dependence of the magnetic anisotropy energy is solely due to spin wave excitations which manifest themselves in the T-dependence of (4) rather than due to thermal expansion or phononic interactions. In other words, there is no additional T-dependence of the parameters K_2, g_0 to be considered in order to describe the non-magnonic effects.

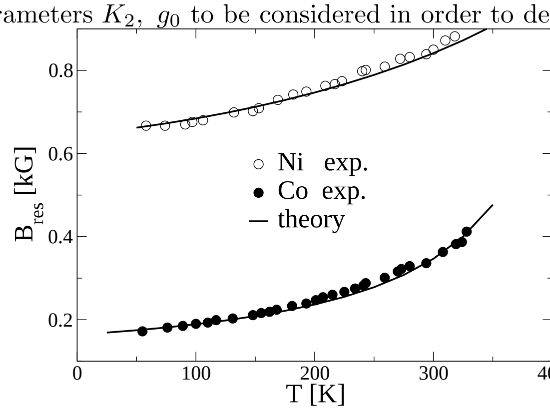

FIG. 4: Full temperature dependence of the resonance field in the easy direction ($\theta_{B_0} = 90°$). Circles are experimental data, lines are from theory with the same parameters as in Fig. 2 and Fig. 3.

In conclusion we presented a quantum theory for thin metallic films based on a local-moment model with lattice and shape anisotropy. By comparison with FMR experiments we found that the temperature dependence of the magnetic anisotropy energy of thin Ni and Co films is exclusively due to magnon excitations rather than caused by other structural or phononic effects.

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[8] These values are larger than the magnetic moments of Ni and Co might suggest. However the crucial quantities in our theory are $JS(S+1)$, $K_2(2S-1)$, g_0S and thus scaling S can be absorbed into the other parameters.